Using Conda Environments on NAS Systems

We provide multiple conda environments for you to use for your machine learning projects. The environments are available via the conda module in the /swbuild/analytix/tools/modulefiles directory.

All of the available environments include the basic machine learning packages, as well as common image processing and natural language processing packages. You can activate the environments via an interactive session or with a PBS batch job.

For a list of environments we currently provide, along with the packages they include, see Machine Learning: Overview.

Loading the Module and Activating the Environments in Interactive Mode

First, access and load the miniconda module, which provides access to the environment:

% module use -a /swbuild/analytix/tools/modulefiles % module load miniconda3/v4

Then, activate one of the environments (where env name is the name of the environment):

- For bash: % source activate env_name
- For csh: % source /swbuild/analytix/tools/miniconda3 220407/bin/activate.csh env name

Useful Conda Commands

After loading the module, you will have access to conda commands, including:

% conda info --envs
Shows available environments.
% conda list -n env_name
Shows installed packages within an environment.
(env_name)% conda deactivate
Deactivates an environment after loading.

For more detailed documentation, see the Conda website.

Using a PBS Batch Job to Activate an Environment

You can activate your machine learning environment, run your program, and deactivate the environment in a PBS script. For example:

```
#!/bin/bash -x

#PBS -I select=1:model=sky_gpu:mpiprocs=1:ncpus=36:ngpus=4:mem=300g

#PBS -I place=scatter:excl

#PBS -q v100

#PBS -I walltime=1:00:00

#PBS -N test

#PBS -j oe

cd $PBS_O_WORKDIR
```

module purge

load the module and environment module -a use /swbuild/analytix/tools/modulefiles module load miniconda3/v4 source activate env_name

run python script python test_cnn.py

deactivate environment conda deactivate

end of script

For more detailed information about running your PBS job on the GPU nodes, see Requesting GPU Resources.

Requesting New or Missing Packages

If you need to use a specific package that is not currently installed in any of the environments, please send an email to support@nas.nasa.gov. In your email, provide the name of the package and request a ticket be opened with the Data Science team. We will help install the package into the existing environments or create a new environment if needed. You can also install your own own conda environment.

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